

## Author Search

⇒ FILE HCAPLUS

FILE 'HCAPLUS' ENTERED AT 13:34:08 ON 28 OCT 2008

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FILE COVERS 1907 - 28 Oct 2008 VOL 149 ISS 18

FILE LAST UPDATED: 27 Oct 2008 (20081027/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

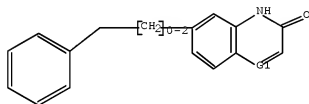
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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

⇒ D STAT QUE L10

L1 STR



G1 C, N

Structure attributes must be viewed using STN Express query preparation.

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L7	209	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	SOMERS	M?/AU
L8	111	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	WOUTERS	W?/AU
L9	430	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	(L4 OR L5 OR L6 OR L7 OR L8)	
L10	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L9 AND L3	

⇒ FILE WPIX

FILE 'WPIX' ENTERED AT 13:34:16 ON 28 OCT 2008  
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FILE LAST UPDATED: 24 OCT 2008 <20081024/UP>  
MOST RECENT UPDATE: 200868 <200868/DW>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE  
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>>> IPC Reform backfile reclassifications have been loaded to end of  
September 2008. No update date (UP) has been created for the  
reclassified documents, but they can be identified by 20060101/UPIC,  
and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC,  
20080401/UPIC, 20080701/UPIC and 20081001/UPIC.  
ECLA reclassifications to mid August and US national classification  
mid September 2008 have also been loaded. Update dates 20080401,  
20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf)

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE  
<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdates/>

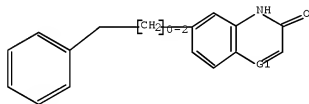
EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:  
[http://www.stn-international.com/archive/presentations/DWPIAnaVist2\\_0608.pdf](http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0608.pdf)

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

⇒ D STAT QUE L16

L1 STR



Structure attributes must be viewed using STN Express query preparation.

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L6	48	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	DUN J?/AU
L7	209	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	SOMERS M?/AU
L8	111	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	WOUTERS W?/AU
L13	4	SEA	FILE=WPIX	SSS	FUL	L1
L14	1	SEA	FILE=WPIX	ABB=ON	PLU=ON	L13/DCR
L15	156	SEA	FILE=WPIX	ABB=ON	PLU=ON	(L4 OR L5 OR L6 OR L7 OR L8)
L16	1	SEA	FILE=WPIX	ABB=ON	PLU=ON	L15 AND L14

⇒ DUP REM L10 L16

FILE 'HCAPLUS' ENTERED AT 13:34:27 ON 28 OCT 2008  
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FILE 'WPIX' ENTERED AT 13:34:27 ON 28 OCT 2008  
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PROCESSING COMPLETED FOR L10  
PROCESSING COMPLETED FOR L16  
L22 2 DUP REM L10 L16 (1 DUPLICATE REMOVED)  
ANSWERS '1-2' FROM FILE HCAPLUS

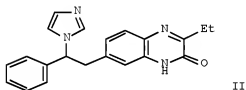
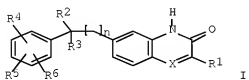
⇒ D IBIB ED ABS HITSTR L22 1-2

L22 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 2005:523429 HCAPLUS Full-text  
DOCUMENT NUMBER: 143:60002  
TITLE: Preparation of 7-phenylalkyl substituted  
2-quinolinones and 2-quinoxalinones as  
poly(ADP-ribose) polymerase inhibitors  
INVENTOR(S): Mabire, Dominique Jean-pierre;  
Guillemont, Jerome Emile Georges; Van Dun,  
Jacobus Alphonsus Josephus; Somers, Maria  
Victorina Francisca; Wouters, Walter  
Boudewijn Leopold  
PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.  
SOURCE: PCT Int. Appl., 55 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005054209	A1	20050616	WO 2004-EP13162	20041118
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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CA 2546002	A1	20050616	CA 2004-2546002	20041118
EP 1709011	A1	20061011	EP 2004-819600	20041118
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU			
CN 1882549	A	20061220	CN 2004-80034287	20041118
BR 2004016817	A	20070306	BR 2004-16817	20041118
JP 2007513087	T	20070524	JP 2006-540337	20041118
US 20080249099	A1	20081009	US 2006-595882	20060517
IN 2006DN02810	A	20070803	IN 2006-DN2810	20060518

MX 2006PA05686	A	20060817	MX 2006-PA5686	20060519
NO 2006002892	A	20060809	NO 2006-2892	20060620
PRIORITY APPLN. INFO.:			EP 2003-78650	A 20031120
			WO 2004-EP13162	W 20041118

OTHER SOURCE(S): CASREACT 143:60002; MARPAT 143:60002  
 ED Entered SIN: 17 Jun 2005  
 GI



AB The title compds. I [ $n = 0-2$ ;  $X = N$ , CR7;  $R7 = H$  or taken together with  $R1$  may form  $CH:CHCH:CH$ ;  $R1 = \text{alkyl, thienyl}$ ;  $R2 = H, OH, \text{alkyl, alkynyl}$  or taken together with  $R3$  may form  $O$ ;  $R3 = OH, OR10, SR11, \text{etc.}$ ;  $R10 = \text{alkyl, alkylcarbonyl, dialkylaminoalkyl}$ ;  $R11 = \text{dialkylaminoalkyl}$ ;  $R4-R6 = H, \text{halo, trihalomethyl, etc.}$ ; with the provision], useful for the treatment of a PARP mediated disorder, were prepared E.g., a multi-step synthesis of II, starting from  $N-[4-(2\text{-oxo-2-phenylethyl})phenyl]acetamide$ , was given. The exemplified compds. I were tested in an in vitro assay based on SPA technol. And in an in vitro filtration assay assessing PARP-1 activity (data given). The pharmaceutical composition comprising the compound I is disclosed.

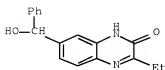
IT 854397-87-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 7-phenylalkyl substituted 2-quinolinones and 2-quinoxalinones as poly(ADP-ribose) polymerase inhibitors)

RN 854397-87-8 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-(hydroxyphenylmethyl)- (CA INDEX NAME)



IT 130347-24-9P 854397-78-7P 854397-82-3P

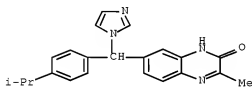
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 854398-17-7P 854398-21-3P 854398-25-7P  
 854398-28-0P 854398-32-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 7-phenylalkyl substituted 2-quinolinones and 2-quinoxalinones as poly(ADP-ribose) polymerase inhibitors)

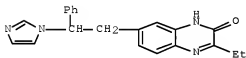
RN 130347-24-9 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl[4-(1-methylethyl)phenyl]methyl]-3-methyl- (CA INDEX NAME)



RN 854397-78-7 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[2-(1H-imidazol-1-yl)-2-phenylethyl]- (CA INDEX NAME)



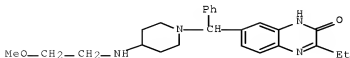
RN 854397-82-3 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[[4-[(2-methoxyethyl)amino]-1-piperidinyl]phenylmethyl]-, ethanedioate (1:1) (CA INDEX NAME)

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CRN 854397-81-2

CMF C25 H32 N4 O2

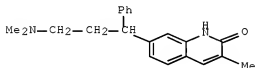


CM 2

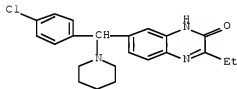
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CMF C2 H2 O4



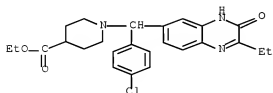
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CN 2 (1H)-Quinolinsonone, 7-[3-(dimethylamino)-1-phenylpropyl]-3-methyl- (CA INDEX NAME)



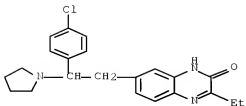
RN 854397-90-3 HCAPLUS  
CN 2 (1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1-piperidinylmethyl]-3-ethyl- (CA INDEX NAME)



RN 854397-92-5 HCAPLUS  
CN 4-Piperidinecarboxylic acid, 1-[(4-chlorophenyl) (2-ethyl-3,4-dihydro-3-oxo-6-quinoxalinylyl)methyl]-, ethyl ester (CA INDEX NAME)



RN 854397-94-7 HCAPLUS  
CN 2 (1H)-Quinoxalinone, 7-[2-(4-chlorophenyl)-2-(1-pyrrolidinyl)ethyl]-3-ethyl- (CA INDEX NAME)



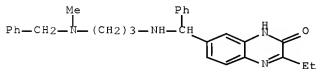
RN 854398-00-8 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[[[3-(methyl(phenylmethyl)amino)propyl]amino]phenylmethyl]-, ethanedioate (1:1)  
(CA INDEX NAME)

CM 1

CRN 854397-99-2

CMF C28 H32 N4 O



CM 2

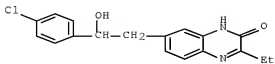
CRN 144-62-7

CMF C2 H2 O4



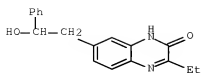
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CN 2(1H)-Quinoxalinone, 7-[2-(4-chlorophenyl)-2-hydroxyethyl]-3-ethyl- (CA INDEX NAME)



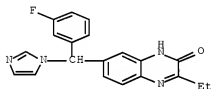
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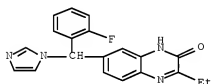
RN 854398-09-7 HCAPLUS

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(CA INDEX NAME)



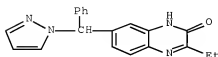
RN 854398-13-3 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[(2-fluorophenyl)-1H-imidazol-1-ylmethyl]-  
(CA INDEX NAME)



RN 854398-17-7 HCAPLUS

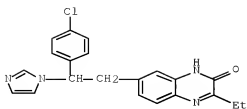
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NAME)



RN 854398-21-3 HCAPLUS

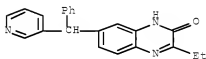
CN 2(1H)-Quinoxalinone, 7-[2-(4-chlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-3-  
ethyl- (CA INDEX NAME)





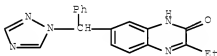
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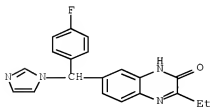
RN 854398-28-0 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-(phenyl-1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)



RN 854398-32-6 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)



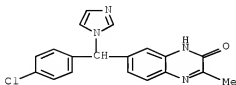
IT 130346-67-7 130346-70-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of 7-phenylalkyl substituted 2-quinolinones and

2-quinoxalinones as poly(ADP-ribose) polymerase inhibitors)

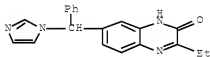
RN 130346-67-7 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-  
(CA INDEX NAME)



RN 130346-70-2 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX  
NAME)



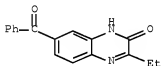
IT 854398-62-2P 854398-71-3P 854398-92-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of 7-phenylalkyl substituted 2-quinolinones and  
2-quinoxalinones as poly(ADP-ribose) polymerase inhibitors)

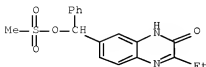
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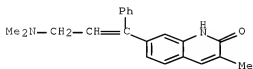


RN 854398-71-3 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-[(methylsulfonyl)oxyphenylmethyl]- (CA  
INDEX NAME)



RN 854398-92-8 HCAPLUS  
 CN 2(1H)-Quinolinone, 7-[3-(dimethylamino)-1-phenyl-1-propen-1-yl]-3-methyl-  
 (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:523424 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 143:60001  
 TITLE: Preparation of 6-alkenyl and 6-phenylalkyl substituted  
 2-quinolinones and 2-quinoxalinones as  
 poly(ADP-ribose) polymerase inhibitors  
 INVENTOR(S): Mabire, Dominique Jean-pierre;  
 Guillemont, Jerome Emile Georges; Van Dun,  
 Jacobus Alphonsus Josephus; Somers, Maria  
 Victorina Francisca; Wouters, Walter  
 Boudewijn Leopold  
 PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.  
 SOURCE: PCT Int. Appl., 102 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054201	A1	20050616	WO 2004-EP13163	20041118
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CN 1882547	A	20061220	CN 2004-80034176	20041118
BR 2004016206	A	20061226	BR 2004-16206	20041118

JP 2007511574	T	20070510	JP 2006-540338	20041118
US 20070072842	A1	20070329	US 2006-595891	20060518
IN 2006DN02813	A	20070803	IN 2006-DN2813	20060518
MX 2006PA05687	A	20060817	MX 2006-PA5687	20060519
NO 2006002894	A	20060809	NO 2006-2894	20060620

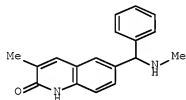
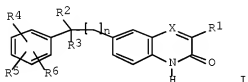
PRIORITY APPLN. INFO.:

WO 2003-EP13028	A	20031120
EP 2003-78860	A	20031205
WO 2003-EP130	A	20031120
WO 2004-EP13163	W	20041118

OTHER SOURCE(S): CASREACT 143:60001; MARPAT 143:60001

ED Entered STN: 17 Jun 2005

GI



AB The title compds. I [n = 0-2; X = N, CR7; R7 = H or taken together with R1 may form CH:CHCH:CH; R1 = alkyl, thiophenyl; R2 = H, OH, alkyl, alkynyl or taken together with R3 may form O; R3 = OH, OR10, SR11, etc.; R10, R11 = CHO, alkyl, (alkyl)amino, etc.; R4-R6 = H, halo, trihalomethyl, etc.; with the provision], useful for the treatment of a PARP mediated disorder, were prepared E.g., a multi-step synthesis of II, starting from bromobenzene and 3-methyl-6-quinolinecarboxaldehyde, was given. The exemplified compds. I were tested in an in vitro assay based on SPA technol. And in an in vitro filtration assay assessing PARP-1 activity (data given). The pharmaceutical composition comprising the compound I is disclosed.

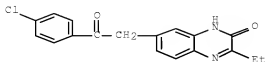
IT 854534-70-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 6-alkenyl and 6-phenylalkyl substituted 2-quinolinones and 2-quinoxalinones as poly(ADP-ribose) polymerase inhibitors)

RN 854534-70-6 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[2-(4-chlorophenyl)-2-oxoethyl]-3-ethyl- (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

# Structure Search

=> FILE HCAPLUS  
FILE 'HCAPLUS' ENTERED AT 13:34:45 ON 28 OCT 2008  
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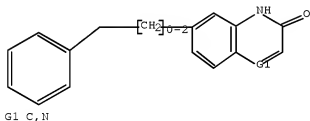
FILE COVERS 1907 - 28 Oct 2008 VOL 149 ISS 18  
FILE LAST UPDATED: 27 Oct 2008 (20081027/ED)

HCaplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.  
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D STAT QUE L3  
L1 STR



Structure attributes must be viewed using STN Express query preparation.  
L2 108 SEA FILE=REGISTRY SSS FUL L1  
L3 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L2

=> S L3 NOT L10  
L23 11 L3 NOT L10

=> FILE WPIX  
FILE 'WPIX' ENTERED AT 13:35:03 ON 28 OCT 2008  
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FILE LAST UPDATED: 24 OCT 2008 <20081024/UP>

MOST RECENT UPDATE: 200868 <200868/DW>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE  
>>> Now containing more than 1.2 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to end of September 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC, and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC, 20080401/UPIC, 20080701/UPIC and 20081001/UPIC.  
ECLA reclassifications to mid August and US national classification mid September 2008 have also been loaded. Update dates 20080401, 20080701 and 20081001/UPEC and /UPNC have been assigned to these. <<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf)

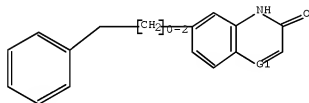
FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE  
<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdates/>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:  
[http://www.stn-international.com/archive/presentations/DWPIAnaVist2\\_0608.pdf](http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0608.pdf)

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D STAT QUE L14  
L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

L13 4 SEA FILE=WPIX \$\$\$ FUL L1  
L14 1 SEA FILE=WPIX ABB=ON PLU=ON L13/DCR

=> S L14 NOT L16  
L24 0 L14 NOT L16

=> FILE BEILSTEIN  
FILE 'BEILSTEIN' ENTERED AT 13:35:19 ON 28 OCT 2008  
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FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.

\*\*\* FILE CONTAINS 10.322,808 SUBSTANCES \*\*\*

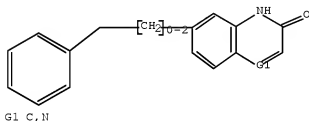
>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

=> D STAT QUE L21  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

L2 108 SEA FILE=REGISTRY SSS FUL L1  
L18 3 SEA FILE=BEILSTEIN ABB=ON PLU=ON L2  
L20 1 SEA FILE=BABS ABB=ON PLU=ON 5711440/BABSAN  
L21 2 SEA FILE=BEILSTEIN ABB=ON PLU=ON L18 NOT L20

=> FILE BABS

FILE 'BABS' ENTERED AT 13:35:33 ON 28 OCT 2008  
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FILE LAST UPDATED: 14 JUL 2008 <20080714/UP>  
FILE COVERS 1980 TO DATE.

=> D STAT QUE L20  
L20 1 SEA FILE=BABS ABB=ON PLU=ON 5711440/BABSAN



=> DUP REM L23 L24 L21 L20  
L24 HAS NO ANSWERS  
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.  
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE  
FILE 'HCAPLUS' ENTERED AT 13:35:55 ON 28 OCT 2008  
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FILE 'BABS' ENTERED AT 13:35:55 ON 28 OCT 2008  
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PROCESSING COMPLETED FOR L23  
PROCESSING COMPLETED FOR L24  
PROCESSING COMPLETED FOR L21  
PROCESSING COMPLETED FOR L20  
L25           13 DUP REM L23 L24 L21 L20 (1 DUPLICATE REMOVED)  
              ANSWERS '1-11' FROM FILE HCAPLUS  
              ANSWERS '12-13' FROM FILE BEILSTEIN

=> D IBIB ED ABS HITSTR 1-11; D IDE ALLREF 12-13

L25 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1  
ACCESSION NUMBER:       1992:592207 HCAPLUS Full-text  
DOCUMENT NUMBER:       117:192207  
ORIGINAL REFERENCE NO.: 117:33223a,33226a  
TITLE:               Fluorine-19 NMR studies on the mechanism of riboflavin  
                      synthase. Synthesis of  
                      6-(trifluoromethyl)-7-oxo-8-(D-ribityl)lumazine and  
                      6-(trifluoromethyl)-7-methyl-8-(D-ribityl)lumazine  
AUTHOR(S):             Cushman, Mark; Patel, Hemantkumar H.; Scheuring,  
                      Johannes; Bacher, Adelbert  
CORPORATE SOURCE:       Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette,  
                      IN, 47907, USA  
SOURCE:                Journal of Organic Chemistry (1992), 57(21), 5630-43  
                      CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE:         Journal  
LANGUAGE:              English  
ED   Entered STN:   15 Nov 1992  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title oxo-(D-ribityl)lumazine I was synthesized by reaction of Me trifluoropyruvate with 5-amino-6-(D-ribitylamino)pyrimidine-2,4(1H,3H)-dione hydrochloride and utilized as a 19F NMR probe of the light riboflavin synthase of *Bacillus subtilis*. I was found to be an inhibitor of riboflavin synthase with an inhibition constant  $K_I = 55 \mu\text{M}$ . The enzyme-bound ligand gave rise to several broad 19F NMR signals which were shifted to low field. The bound ligand I could be displaced from the enzyme by the enzyme product, riboflavin (II), and the product analog, 5-nitroso-6-(ribitylamino)-2,4(1H,3H)-pyrimidinedione. Title methyl-(D-ribityl)lumazine III was synthesized by reaction of 5-amino-6-(D-ribitylamino)pyrimidine-2,4(1H,3H)-dione hydrochloride with 1,1,1-trifluorobutane-2,3-dione. Three mols. of III can be

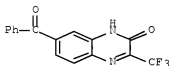
bound relatively tightly per mol of riboflavin synthase, i.e., one ligand mol. per protein subunit. A scheme for the catalytic cycle of riboflavin synthase is proposed.

IT 143309-80-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 143309-80-2 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-benzoyl-3-(trifluoromethyl)- (CA INDEX NAME)



L25 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1101739 HCAPLUS Full-text

DOCUMENT NUMBER: 149:355743

TITLE: Quinolinone derivatives as PARP and TANK inhibitors and their preparation, pharmaceutical compositions and use in the treatment of diseases

INVENTOR(S): Vialard, Jorge Eduardo; Angibaud, Patrick Rene; Mevellec, Laurence Anne; Meyer, Christophe; Freyne, Eddy Jean Edgard; Pilatte, Isabelle Noelle Constance; Roux, Bruno; Pasquier, Elisabeth Therese Jeanne; Bourdrez, Xavier Marc; Adelinet, Christophe Denis; Marconnet-Decrane, Laurence Francoise Bernadette; Macritchie, Jacqueline Anne; Duffy, James Edward Stewart; Owens, Andrew Pate; Storck, Pierre-Henri; Poncelet, Virginie Sophie

PATENT ASSIGNEE(S): Janssen Pharmaceutica NV, Belg.

SOURCE: PCT Int. Appl., 223pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

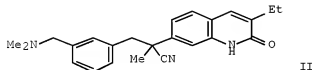
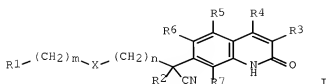
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008107478	A1	20080912	WO 2008-EP52764	20080307
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: EP 2007-103788 A 20070308  
US 2007-893680P P 20070308



AB The invention provides compds. of formula I, their use as PARP inhibitors as well as pharmaceutical compns. comprising said compds. Compds. of formula I wherein m is 0, 1 and 2 when N is 0; n is 0, 1, 2, 3 and 4 when m is 0; X is a bond, (un)substituted methylene; CONH and derivs., NH and derivs., O, and C.tplbond.C; R1 is (un)substituted (hetero)aryl; R2 is H, Me, Et, Pr, C3-6 cycloalkyl(methyl), F, Ph, cyanophenyl, and CF3; R3 is Me, Et, Pr, HOCH2, halo, CF3, MeO and C1-6 alkylcarbonyl; R4 is H, halo, Me, (hydroxy)aminocarbonyl, etc.; R5, R5 and R7 are independently H, halo, C1-6 alkoxy, CN, C1-6 alkyl, OCH2CH2NH2 and derivs., etc.; and their N-oxides, pharmaceutically acceptable addition salts, stereochem. isomeric forms thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their PARP and TANK inhibitory activity (data given).

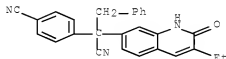
IT 1056887-62-7E 1056887-63-8E

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinoline derivs. as PARP and TANK inhibitors useful in the treatment of diseases)

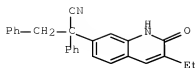
RN 1056887-62-7 HCAPLUS

CN 7-Quinolineacetoneitrile,  $\alpha$ -(4-cyanophenyl)-3-ethyl-1,2-dihydro-2-oxo- $\alpha$ -(phenylmethyl)- (CA INDEX NAME)



RN 1056887-63-8 HCAPLUS

CN 7-Quinolineacetoneitrile, 3-ethyl-1,2-dihydro-2-oxo- $\alpha$ -phenyl- $\alpha$ -(phenylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:565829 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:422287

TITLE: A very efficient synthesis of (1H)-1,5-diazaanthracene-2,9,10-triones

AUTHOR(S): Ubeda, J. Ignacio; Villacampa, Mercedes; Avendano, Carmen

CORPORATE SOURCE: Departamento de Quimica Organica y Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain

SOURCE: Letters in Organic Chemistry (2005), 2(4), 374-377

CODEN: LOCEC7; ISSN: 1570-1786

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:422287

ED Entered STN: 30 Jun 2005

AB Acylation of ortho-lithiated species derived from N,O-dipivaloyl-6-amino-5,8-dimethoxy-4-methyl-2(1H)-quinolinone, followed by condensation with carbonyl reagents and in situ N-deprotection gave 7-alkyl- or 6,7-dialkyl-9,10-dimethoxy-4-methyl-1,5-diaza-2(1H)-anthracenones, which were finally oxidized to the title compds.

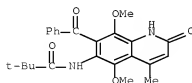
IT 868289-13-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diazaanthracenetriones via acylation of aminoquinolinones and subsequent cyclocondensation with carbonyl compds.)

RN 868289-13-8 HCAPLUS

CN Propanamide, N-(7-benzoyl-1,2-dihydro-5,8-dimethoxy-4-methyl-2-oxo-6-quinolinyl)-2,2-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:430796 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:7139

TITLE: Preparation of indolylquinoxalones for treating hyperproliferative disorders and diseases associated with angiogenesis

INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng; Brittelli, David R.; Burke, Michael J.; Chen, Gang; Cook, James; Dumas, Jacques; Sibley, Robert; Turner, Michael R.

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

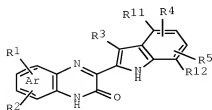
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043950	A1	20040527	WO 2003-US36003	20031110
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RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2505819	A1	20040527	CA 2003-2505819	20031110
AU 2003290744	A1	20040603	AU 2003-290744	20031110
EP 1565455	A1	20050824	EP 2003-783328	20031110
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003016169	A	20050927	BR 2003-16169	20031110
CN 1738814	A	20060222	CN 2003-80108639	20031110
JP 2006509840	T	20060323	JP 2005-507146	20031110
MX 2005PA04779	A	20050722	MX 2005-PA4779	20050504
US 20060004011	A1	20060105	US 2005-534215	20050506
NO 2005002796	A	20050609	NO 2005-2796	20050609
PRIORITY APPLN. INFO.:			US 2002-425490P	P 20021112
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			US 2003-484202P	P 20030630
			WO 2003-US36003	W 20031110

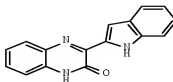
OTHER SOURCE(S): MARPAT 141:7139

ED Entered STN: 27 May 2004

GI



I



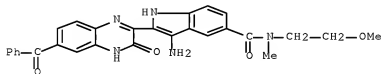
II

AB The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF<sub>3</sub>, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO<sub>2</sub>, NH<sub>2</sub>, alkylamino, alkoxyamino, or (un)substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%).

IT 694531-90-3P 694531-94-7P 694532-29-1P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (antiproliferative and angiogenesis inhibitor; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

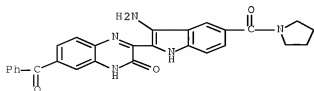
RN 694531-90-3 HCAPLUS

CN 1H-Indole-5-carboxamide, 3-amino-2-(6-benzoyl-3,4-dihydro-3-oxo-2-quinoxalinyl)-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)



RN 694531-94-7 HCAPLUS

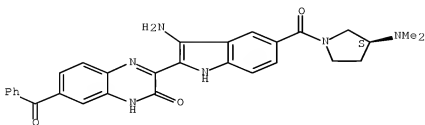
CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(1-pyrrolidinylcarbonyl)-1H-indol-2-yl]-7-benzoyl- (CA INDEX NAME)



RN 694532-29-1 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-[[[(3S)-3-(dimethylamino)-1-pyrrolidinyl]carbonyl]-1H-indol-2-yl]-7-benzoyl- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:482884 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:239238

TITLE: A novel quinoline alkaloid possessing a 7-benzyl group from the centipede, Scolopendra subspinipes

AUTHOR(S): Noda, Naoki; Yashiki, Yuji; Nakatani, Takafumi;

Miyahara, Kazumoto; Du, Xiao-Ming

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Setsunan

University, Osaka, 573-0101, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2001), 49(7), 930-931

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 05 Jul 2001

AB The novel quinoline alkaloid scolopendrine was isolated from the centipede, Scolopendra subspinipes mutilans L. Koch. The structure was determined to be 2-hydroxy-7-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-8-quinolyl sulfate on the basis of high-resolution electron-spray ionization mass spectroscopy and two-dimensional NMR spectral data. Unlike quinoline alkaloids so far reported, scolopendrine is unique in having a 7-benzyl moiety in the quinoline ring.

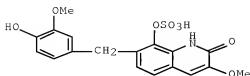
IT 360550-09-0, Scolopendrine

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); RACT (Reactant or reagent)

(quinoline alkaloid from Scolopendra subspinipes)

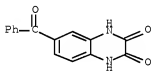
RN 360550-09-0 HCAPLUS

CN 2(1H)-Quinolinone, 7-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-8-(sulfoxy)- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2001:223060 HCAPLUS Full-text  
DOCUMENT NUMBER: 135:5590  
TITLE: Some nucleophilic reactions with  
6-benzoyl-2,3-dichloroquinoxaline: synthesis of  
tetrazolo[1,5-a]quinoxaline,  
2-methylidene-1,3-dithiolo[4,5-b]quinoxalines,  
quinoxalino[2,3-b]quinoxalines and  
pyrazolo[1',5':1,2]imidazolo[4,5-b]-quinoxalines  
AUTHOR(S): El-Gaby, M. S. A.; El-Sharief, A. M. Sh; Ammar, Y. A.;  
Mohamed, Y. A.; El-Salam, A. A. Abd  
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Al-Azhar  
University at Assiut, Assiut, 71524, Egypt  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (2001),  
40B(3), 195-200  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: National Institute of Science Communication, CSIR  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 135:5590  
ED Entered STN: 29 Mar 2001  
AB The starting material 6-benzoyl-2,3-dichloroquinoxaline is subjected to some  
nucleophilic reagents to study the effect of the benzoyl group on the  
reactivity of the two chlorine atoms.  
IT 143702-68-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactions of 6-benzoyl-2,3-dichloroquinoxaline with nucleophiles)  
RN 143702-68-5 HCAPLUS  
CN 2,3-Quinoxalinedione, 6-benzoyl-1,4-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2000:527827 HCAPLUS Full-text  
DOCUMENT NUMBER: 134:162992  
TITLE: Synthesis and antimicrobial activities of some novel  
quinoxalinone derivatives  
AUTHOR(S): Ali, M. M.; Ismail, M. M. F.; El-Gaby, M. S. A.;  
Zahran, M. A.; Ammar, Y. A.  
CORPORATE SOURCE: Dep. of Chemistry, Faculty of Science, Al-Azhar Univ.,  
Cairo, 11884, Egypt  
SOURCE: Molecules [online computer file] (2000), 5(6), 864-873



CODEN: MOLEFW; ISSN: 1420-3049

URL: <http://www.mdpi.org/molecules/papers/50600864.pdf>

PUBLISHER:

Molecular Diversity Preservation International

DOCUMENT TYPE:

Journal; (online computer file)

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 134:162992

ED Entered STN: 03 Aug 2000

GI



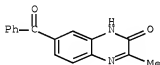
AB Condensation of 4-benzoyl-1,2-phenylenediamine with sodium pyruvate in acetic acid furnished two products, which were identified as 6-benzoyl- (I) and 7-benzoyl-3-methyl-2(1H)-quinoxalinone (II). Fusion of I with aromatic aldehydes furnished the styryl derivs. Alkylation of I and II with di-Me sulfate or Et chloroacetate produced the N-alkyl derivs. Hydrazinolysis of one ester derivative with hydrazine hydrate afforded the hydrazide derivative, which underwent condensation with aldehydes to give the corresponding hydrazone derivs. In addition, chlorination of I with thionyl chloride afforded the 2-chloro derivative, which was subjected to reaction with sodium azide and n-butylamine to yield the corresponding tetrazolo (III) and n-butylamino (IV) derivs., resp. The structures of the compds. prepared were confirmed by anal. and spectral data. Also, some of the synthesized compds. were screened for antimicrobial activity.

IT 325469-52-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation and antimicrobial activities of quinoxalinone derivs.)

RN 325469-52-1 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-benzoyl-3-methyl- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:82353 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 132:273870

TITLE: Discovery of novel HIV-1 reverse transcriptase inhibitors using a combination of 3D database searching and 3D QSAR

AUTHOR(S): Zaharevitz, Daniel W.; Gussio, Rick; Wiegand, Ann; Jalluri, Ravi; Pattabiraman, Nagarajan; Kellogg, Glen E.; Pallansch, Luke A.; Yang, Stringer S.; Buckheit, Robert W., Jr.

CORPORATE SOURCE: Developmental Therapeutics Program, National Cancer Institute, Bethesda, MD, 20892-7444, USA

SOURCE: Medicinal Chemistry Research (1999), 9(7/8), 551-564  
CODEN: MCREEB; ISSN: 1054-2523

PUBLISHER: Birkhaeuser Boston

DOCUMENT TYPE: Journal

LANGUAGE: English

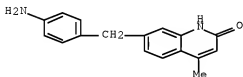
ED Entered STN: 03 Feb 2000

AB 3D searches in a database (National Cancer Institute repository) of over 100,000 compds. were followed by evaluations of hits in a 3D QSAR model for the non-nucleoside binding site of HIV-1 reverse transcriptase. The procedure resulted in the identification of a set of novel and structurally diverse inhibitors and required testing of only 225 compds.

IT 261789-30-4, NSC 109817  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(discovery of novel HIV-1 reverse transcriptase inhibitors using a combination of 3D database searching and 3D QSAR)

RN 261789-30-4 HCAPLUS

CN 2(1H)-Quinolinone, 7-[(4-aminophenyl)methyl]-4-methyl- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1992:571381 HCAPLUS Full-text

DOCUMENT NUMBER: 117:171381

ORIGINAL REFERENCE NO.: 117:29633a,29636a

TITLE: Synthesis of pyrido[1',2':1,2]imidazo[4,5-b]quinoxalines

AUTHOR(S): Tanaka, Kiyoshi; Takahashi, Hideki; Takimoto, Kozo; Sugita, Masahiko; Mitsuhashi, Keiyo

CORPORATE SOURCE: Fac. Eng., Seikei Univ., Musahino, 180, Japan

SOURCE: Journal of Heterocyclic Chemistry (1992), 29(4), 771-7  
CODEN: JHTCAD; ISSN: 0022-152X

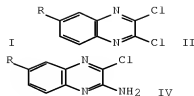
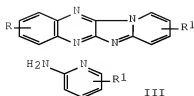
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:171381

ED Entered STN: 01 Nov 1992

GI

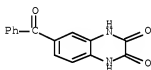


AB Synthesis of title compds. I (R = H, 8-, 9-Cl, 8-, 9-Bz, 8-, 9-NO<sub>2</sub>; R<sub>1</sub> = H, 1-, 2-, 3-, 4-Me, 4-PhCH<sub>2</sub>O) by the facile cyclizations of 2,3-dichloroquinoxalines II with 2-aminopyridines III and of 2-amino-3-chloroquinoxalines IV (R ≠ H) with various substituted pyridines is described.

IT 143702-68-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (chlorination of)

RN 143702-68-5 HCAPLUS

CN 2,3-Quinoxalinedione, 6-benzoyl-1,4-dihydro- (CA INDEX NAME)



L25 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:612014 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 113:212014

ORIGINAL REFERENCE NO.: 113:35835a, 35838a

TITLE: Preparation of (1H-azol-1-ylmethyl)quinolines, -quinazolines, and -quinoxalines as drugs

INVENTOR(S): Freyne, Eddy Jean Edgard; Venet, Marc Gaston; Raeymaekers, Alfons Herman Margaretha; Sanz, Gerard Charles

PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.

SOURCE: Eur. Pat. Appl., 106 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 371564	A2	19900606	EP 1989-203014	19891128
EP 371564	A3	19910529		
EP 371564	B1	19950712		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5028606	A	19910702	US 1989-434957	19891113
US 5037829	A	19910806	US 1989-435120	19891113
CA 2002864	A1	19900529	CA 1989-2002864	19891114
CA 2002864	C	19991116		

DK 8905994	A	19900530	DK 1989-5994	19891128
DK 172748	B1	19990628		
NO 8904734	A	19900530	NO 1989-4734	19891128
NO 174509	B	19940207		
NO 174509	C	19940518		
AU 8945646	A	19900607	AU 1989-45646	19891128
AU 620946	B2	19920227		
HU 52498	A2	19900728	HU 1989-6220	19891128
HU 205106	B	19920330		
ZA 8909076	A	19910731	ZA 1989-9076	19891128
SU 1780536	A3	19921207	SU 1989-4742543	19891128
IL 92486	A	19930708	IL 1989-92486	19891128
ES 2088889	T3	19961001	ES 1989-203014	19891128
FI 101964	B	19980930	FI 1989-5687	19891128
FI 101964	B1	19980930		
CN 1042912	A	19900613	CN 1989-108925	19891129
CN 1033752	C	19970108		
JP 02223579	A	19900905	JP 1989-307793	19891129
JP 2916181	B2	19990705		
US 5151421	A	19920929	US 1991-672298	19910320
US 5185346	A	19930209	US 1991-704746	19910523
US 5268380	A	19931207	US 1992-973871	19921110
US 5441954	A	19950815	US 1993-131817	19931005
CN 1106004	A	19950802	CN 1994-117801	19941102
CN 1036002	C	19971001		
CN 1106005	A	19950802	CN 1994-117802	19941102
CN 1036003	C	19971001		
US 5612354	A	19970318	US 1995-409551	19950323

PRIORITY APPLN. INFO.:

	GB 1988-27820	A	19881129
	GB 1988-27821	A	19881129
	GB 1988-27822	A	19881129
	US 1989-434205	B2	19891113
	US 1989-434957	A3	19891113
	US 1991-704746	A3	19910523
	US 1992-973871	A3	19921110
	US 1993-131817	A3	19931005

OTHER SOURCE(S): MARPAT 113:212014

ED Entered STN: 08 Dec 1990

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; R = H, alkyl; X1:X2 = CH:CH, CH:N, N:CH; Y = H, alkyl, cycloalkyl, alkenyl, alkynyl, (un)substituted aryl, aralkyl; Z = (un)substituted (oxo)quinoliny, (oxo- or thioxo)quinazolinyl, (oxo- or dioxo)quinoxaliny] were prepared as retinoic acid metabolism inhibitors, aromatase inhibitors, etc. Thus, 3,4-dihydroquinolin-2(1H)-one was stirred 2 h at 70° with BzCl in DMF containing AlCl3 and the product reduced by NaBH4 to give hydroxymethylquinolinone II (R1 = Ph, R2 = OH). II (R1 = Me, R2 = OH) was stirred overnight with SOCl2 in THF and the product II (R1 = Me, R2 = Cl) stirred overnight at 60-70° with 1H-imidazole in DMSO to give II (R1 = Me, R2 = imidazo) which maintained plasma levels of i.v. administered all-trans-retinoic acid at ≥10 ng/mL in rats 2 h after oral administration of 40 mg/kg.

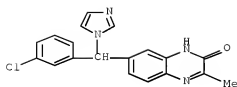
IT 130346-36-0P 130346-36-2P 130346-40-6P  
 130346-50-8P 130346-67-7P 130346-70-2P  
 130346-74-6P 130346-78-0P 130347-24-9P  
 130347-27-2P 130347-29-4P 130347-36-5P  
 130347-40-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as retinoate metabolism and aromatase inhibitor)

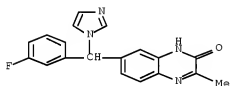
RN 130346-36-0 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-  
 (CA INDEX NAME)



RN 130346-38-2 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[(3-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-  
(CA INDEX NAME)



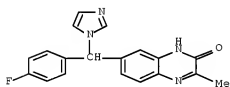
RN 130346-40-6 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-  
, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 130346-39-3

CMF C19 H15 F N4 O



CM 2

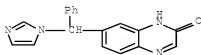
CRN 144-62-7

CMF C2 H2 O4



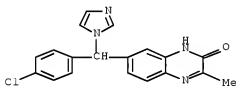
RN 130346-50-8 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)



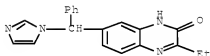
RN 130346-67-7 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl- (CA INDEX NAME)



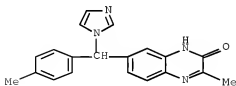
RN 130346-70-2 HCAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)



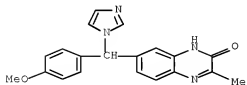
RN 130346-74-6 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl(4-methylphenyl)methyl]-3-methyl- (CA INDEX NAME)



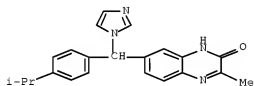
RN 130346-78-0 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl(4-methoxyphenyl)methyl]-3-methyl-  
(CA INDEX NAME)



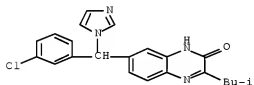
RN 130347-24-9 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl[4-(1-methylethyl)phenyl]methyl]-3-methyl-  
(CA INDEX NAME)



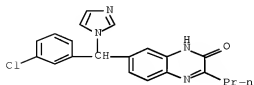
RN 130347-27-2 HCAPLUS

CN 2(1H)-Quinoxalinone, 7-[ (3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(2-methylpropyl)-  
(CA INDEX NAME)

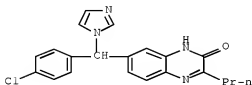


RN 130347-29-4 HCAPLUS

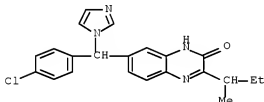
CN 2(1H)-Quinoxalinone, 7-[ (3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl-  
(CA INDEX NAME)



RN 130347-38-5 HCAPLUS  
 CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl-  
 (CA INDEX NAME)

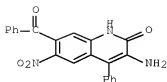


RN 130347-40-9 HCAPLUS  
 CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(1-methylpropyl)- (CA INDEX NAME)



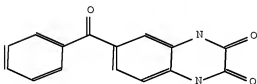
L25 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1974:569519 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 81:169519  
 ORIGINAL REFERENCE NO.: 81:26231a,26234a  
 TITLE: Cyclization of some o-substituted benzophenone derivatives  
 AUTHOR(S): Jaszowska, Anna; Serafin, Barbara  
 CORPORATE SOURCE: Inst. Org. Chem. Technol., Polytech. Univ., Warsaw, Pol.  
 SOURCE: Roczniki Chemii (1974), 48(6), 1029-40  
 CODEN: ROCHAC; ISSN: 0035-7677  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 12 May 1984  
 GI For diagram(s), see printed CA Issue.  
 AB o-Aminobenzophenone oximes were cyclized in AcOH at 50° to quinazoline derivs., which with MeNH2 at -10° gave 1,4-benzodiazepine derivs. (I, R = Cl, Br). II with H2NCH2CH2NH2 gave III (R1 = NO2). III (R1 = Cl) was also prepared The yields were 48-95%.  
 IT 53824-15-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 53824-15-0 HCAPLUS  
 CN 2(1H)-Quinolinone, 3-amino-7-benzoyl-6-nitro-4-phenyl- (CA INDEX NAME)





L25 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	5437606
Beilstein Pref. RN (BPR):	143702-68-5
CAS Reg. No. (RN):	143702-68-5
Chemical Name (CN):	6-benzoyl-1,4-dihydro-quinoxaline-2,3-dione
Autonom Name (AUN):	6-benzoyl-1,4-dihydro-quinoxaline-2,3-dione
Molec. Formula (MF):	C15 H10 N2 O3
Molecular Weight (MW):	266.26
Lawson Number (LN):	28970
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	4781338
Tautomer ID (TAUTID):	5205284
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1993/05/04
Update Date (DUPD):	1994/02/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1

CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

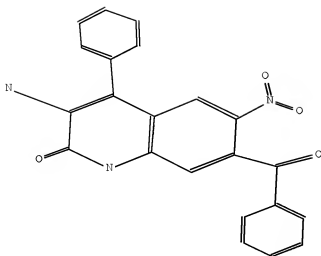
Code	Name	Occurrence
RX	Reaction Documents	1
RXREA	Substance is Reaction Reactant	1

All References:  
ALLREF

1. Tanaka, Kiyoshi; Takahashi, Hideki; Takimoto, Kozo; Sugita, Masahiko; Mitsuhashi, Keiyo, J.Heterocycl.Chem., CODEN: JHTCAD, 29(4), <1992>, 771-777; BABS-5655913

L25 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2008 Elsevier Inf. Sys. on STN

Beilstein Records (BRN):	453719
Beilstein Pref. RN (BPR):	53824-15-0
CAS Reg. No. (RN):	53824-15-0
Chemical Name (CN):	3-amino-7-benzoyl-6-nitro-4-phenyl-1H-quinolin-2-one
Autonom Name (AUN):	3-amino-7-benzoyl-6-nitro-4-phenyl-1H-quinolin-2-one
Molec. Formula (MF):	C22 H15 N3 O4
Molecular Weight (MW):	385.38
Lawson Number (LN):	27776
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	447290
Tautomer ID (TAUTID):	476487
Beilstein Citation (BSO):	5-22-13-00354
Entry Date (DED):	1988/11/28
Update Date (DUPD):	1992/05/13



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:  
ALLREF

1. Jazzkowska, A.; Serafin, B., Roczn.Chem., CODEN: ROCHAC, 48, <1974>, 1029-1040

# Search History

ACT BAE882STR1/A

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STR

L1  
L2 108 SEA SSS FUL L1  
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FILE 'HCAPLUS' ENTERED AT 13:23:11 ON 28 OCT 2008

L3 13 SEA ABB=ON PLU=ON L2  
L4 12 SEA ABB=ON PLU=ON MABIRE D?/AU  
L5 68 SEA ABB=ON PLU=ON GUILLEMONT J?/AU  
L6 48 SEA ABB=ON PLU=ON DUN J?/AU  
L7 209 SEA ABB=ON PLU=ON SOMERS M?/AU  
L8 111 SEA ABB=ON PLU=ON WOUTERS W?/AU  
L9 430 SEA ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8)  
L10 2 SEA ABB=ON PLU=ON L9 AND L3

FILE 'HCAPLUS' ENTERED AT 13:24:16 ON 28 OCT 2008

L11 13 SEA ABB=ON PLU=ON L2

FILE 'WPIX' ENTERED AT 13:25:08 ON 28 OCT 2008

L12 2 SEA SSS SAM L1  
L13 4 SEA SSS FUL L1  
L14 1 SEA ABB=ON PLU=ON L13/DCR  
L15 156 SEA ABB=ON PLU=ON (L4 OR L5 OR L6 OR L7 OR L8)  
L16 1 SEA ABB=ON PLU=ON L15 AND L14

FILE 'BEILSTEIN' ENTERED AT 13:31:27 ON 28 OCT 2008

L17 3 SEA ABB=ON PLU=ON L2  
L18 3 SEA ABB=ON PLU=ON L2  
L19 1 SEA ABB=ON PLU=ON L18 AND BABSAN/FA  
SEL BABSAN

FILE 'BABS' ENTERED AT 13:32:10 ON 28 OCT 2008

L20 1 SEA ABB=ON PLU=ON 5711440/BABSAN

FILE 'BEILSTEIN' ENTERED AT 13:32:19 ON 28 OCT 2008

L21 2 SEA ABB=ON PLU=ON L18 NOT L20

FILE 'HCAPLUS, WPIX' ENTERED AT 13:34:27 ON 28 OCT 2008

L22 2 DUP REM L10 L16 (1 DUPLICATE REMOVED)

FILE 'HCAPLUS' ENTERED AT 13:34:45 ON 28 OCT 2008

L23 11 SEA ABB=ON PLU=ON L3 NOT L10

FILE 'WPIX' ENTERED AT 13:35:03 ON 28 OCT 2008

L24 0 SEA ABB=ON PLU=ON L14 NOT L16

FILE 'HCAPLUS, BEILSTEIN, BABS' ENTERED AT 13:35:55 ON 28 OCT 2008

L25 13 DUP REM L23 L24 L21 L20 (1 DUPLICATE REMOVED)